Halogen bonding or close packing? Examining the structural landscape in a series of Cu(II)-acac complexes

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Supporting Information

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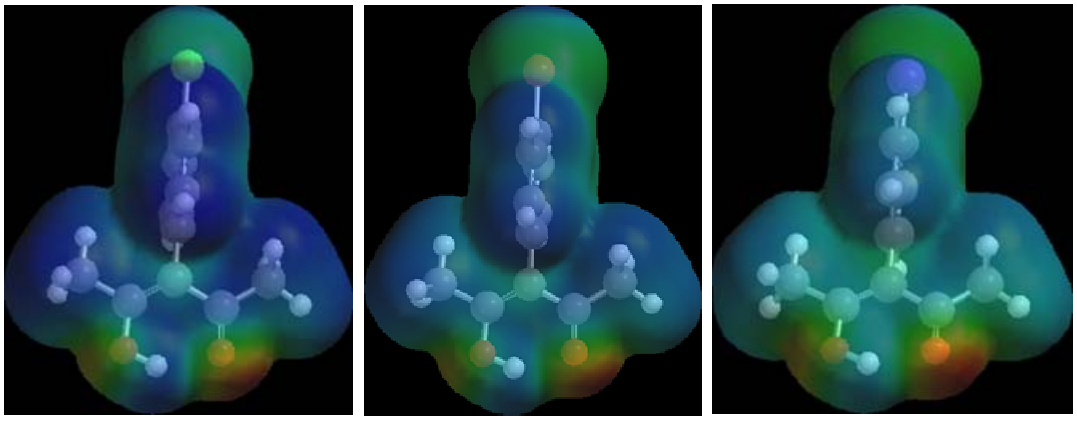
General experimental details

^{1}H NMR spectra were recorded on a Varian Unity plus 400 MHz spectrometer in $CDCl_3$. Data is expressed in parts per million (ppm) downfield shift from tetramethylsilane or residual protiosolvent as internal reference and are reported as position (in ppm), multiplicity (s = singlet, d = doublet, t = triplet, m= multiplet), coupling constant (J in Hz) and integration (number of protons). ^{13}C nuclear magnetic resonance spectra were recorded on a Varian Unity plus 400 MHz spectrometer in $CDCl_3$ with complete proton decoupling. Data is expressed in parts per million (ppm) shift relative to $CDCl_3$ (77.00 ppm) and are reported as position (δ). Melting points were recorded on a Fisher-Johns melting point apparatus and are uncorrected. Infrared spectroscopy (IR) was done on a Nicolet 380 FT-IR. All the chemicals were purchased from Aldrich and used without further purification, unless otherwise noted.

Molecular electrostatic potential charge calculations of 3-5

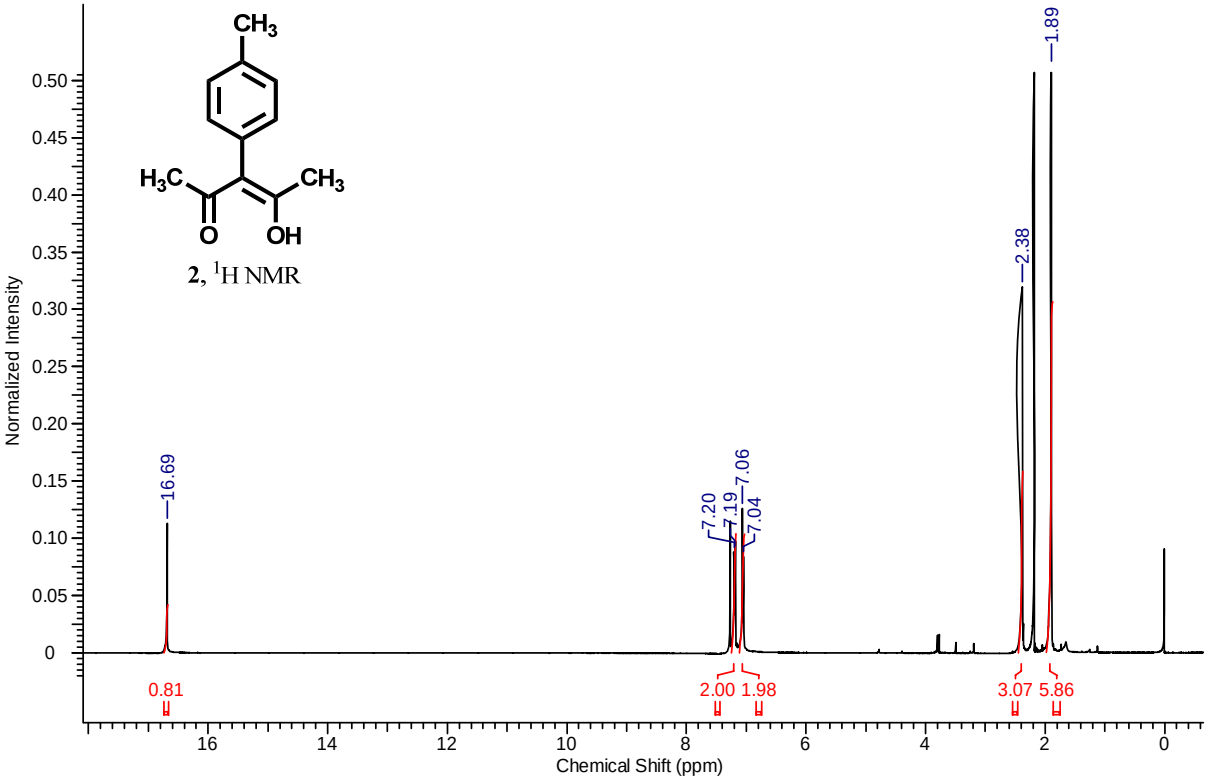
Charge calculations were performed using Spartan'04 (Wavefunction, Inc. Irvine, CA). All three molecules were optimized using PM3, with the maxima and minima in the electrostatic potential surface (0.002 e au^{-1} iso-surface) determined using a positive point charge in the vacuum as a probe.

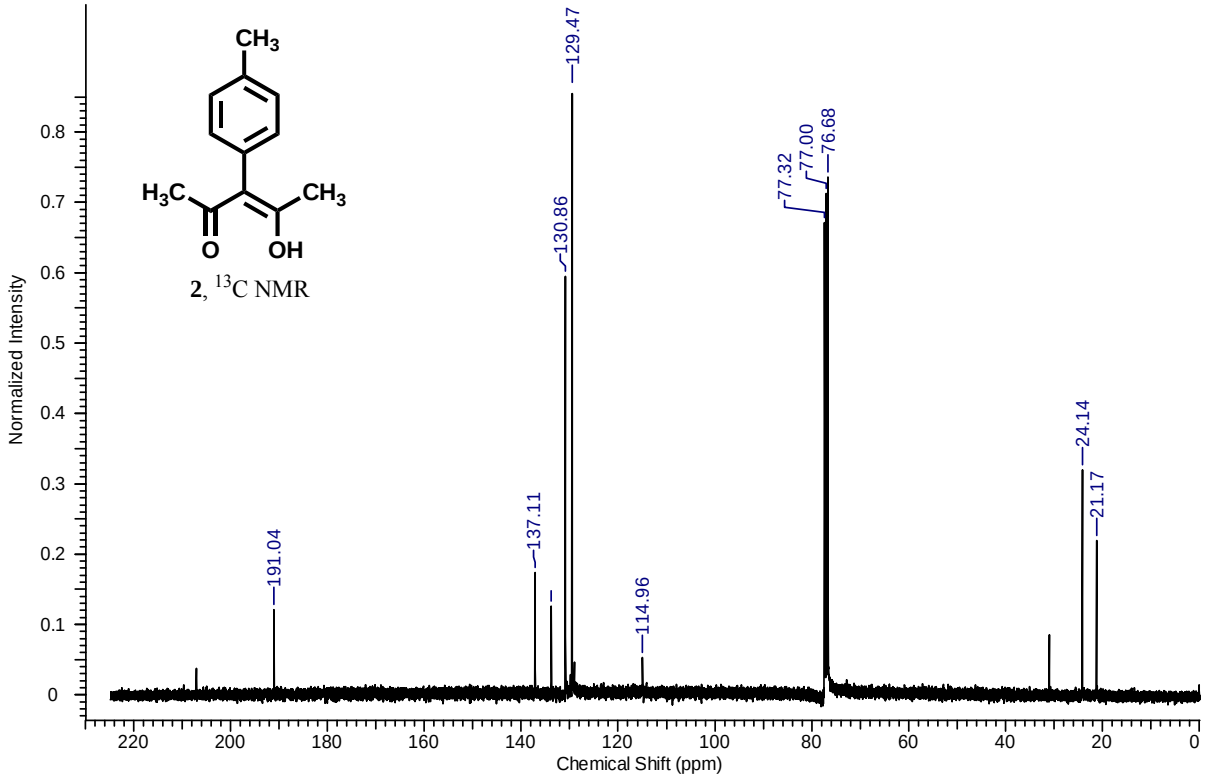


3 **4** **5**

Fig. S1 MEP surface calculations of the ligands **3-5**.

NMR data


CH3
H3C
CH3
O
OH
2, 1H NMR
Normalized Intensity
Chemical Shift (ppm)
16.69
7.20
7.19
7.06
7.04
2.38
1.89
0.81
2.00
1.98
3.07
5.86


CH3
H3C
CH3
O
OH
2, 13C NMR
Normalized Intensity
Chemical Shift (ppm)
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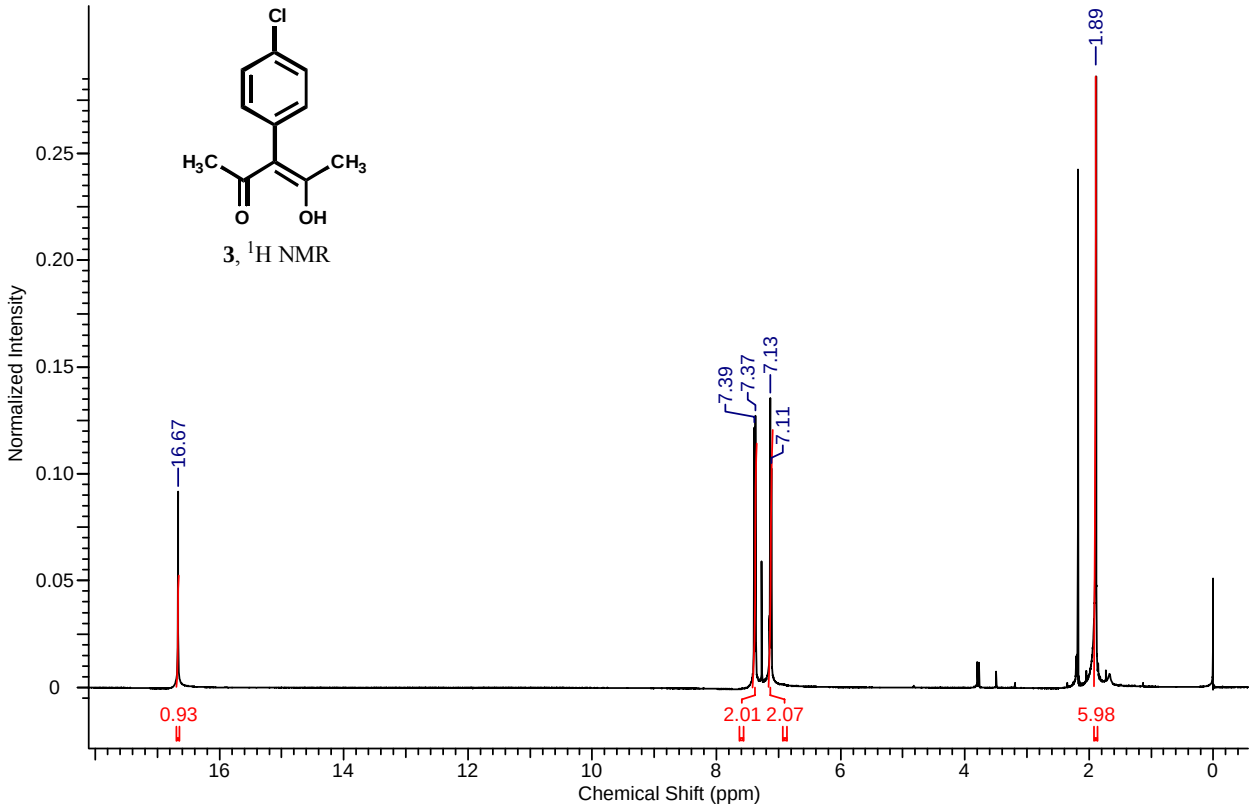
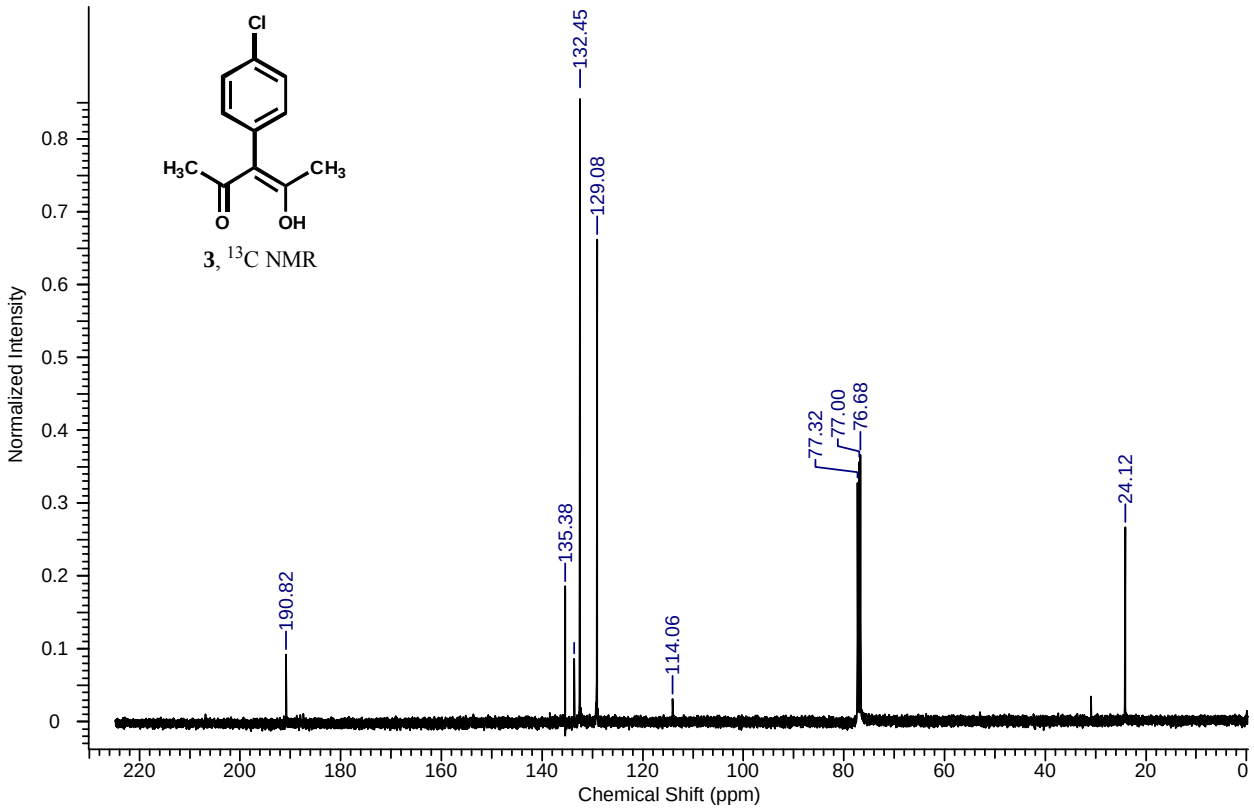
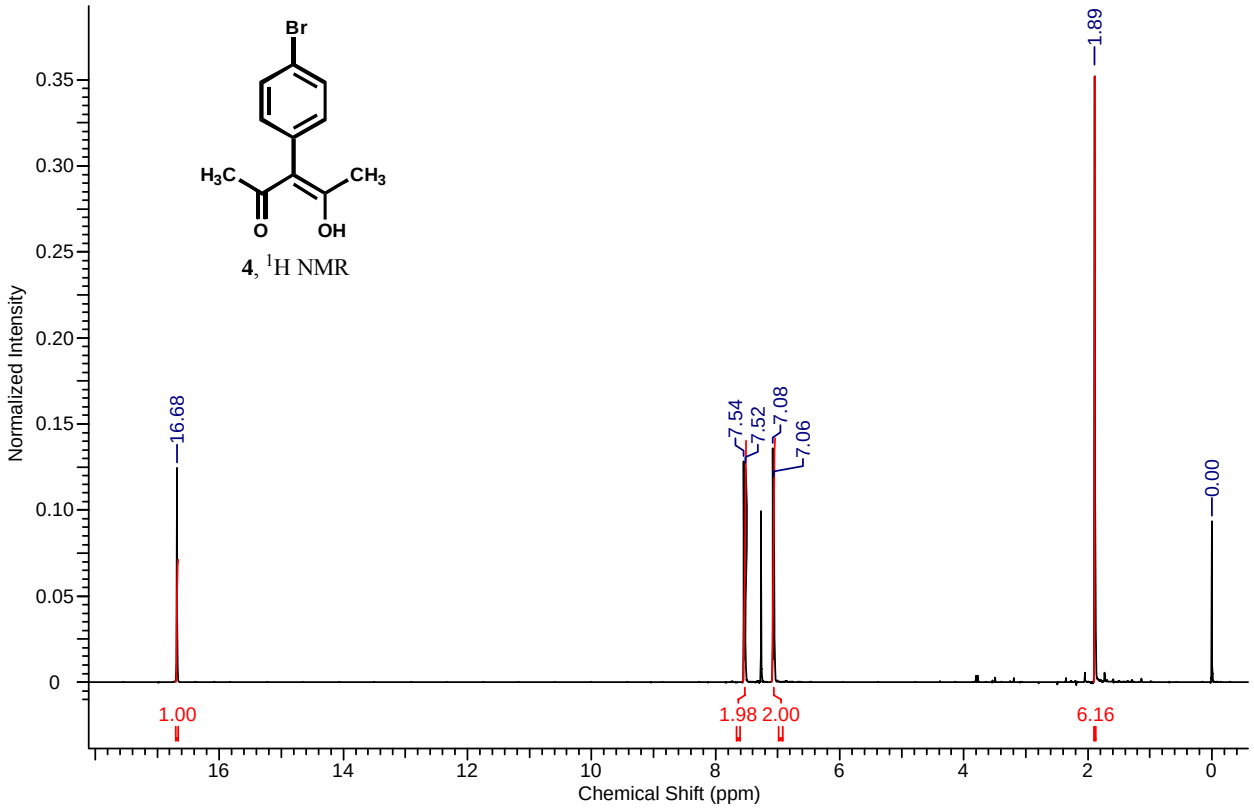
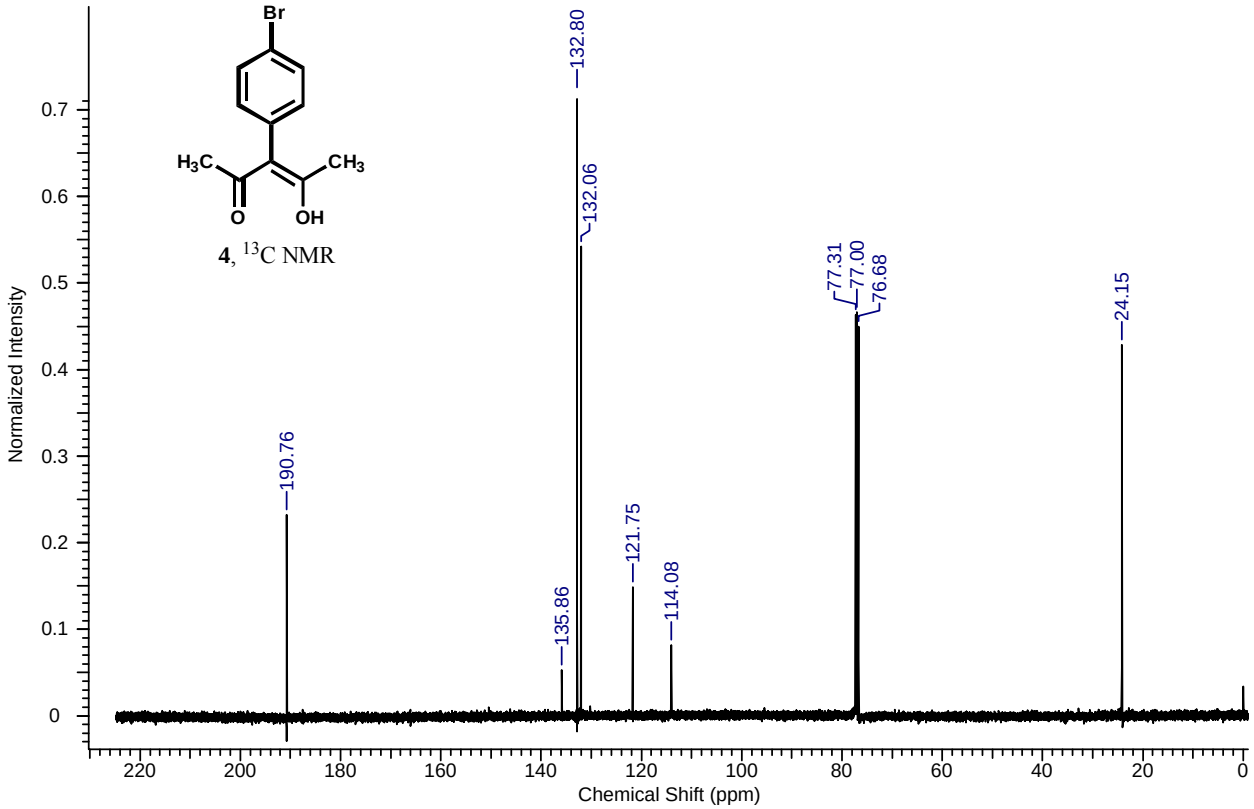
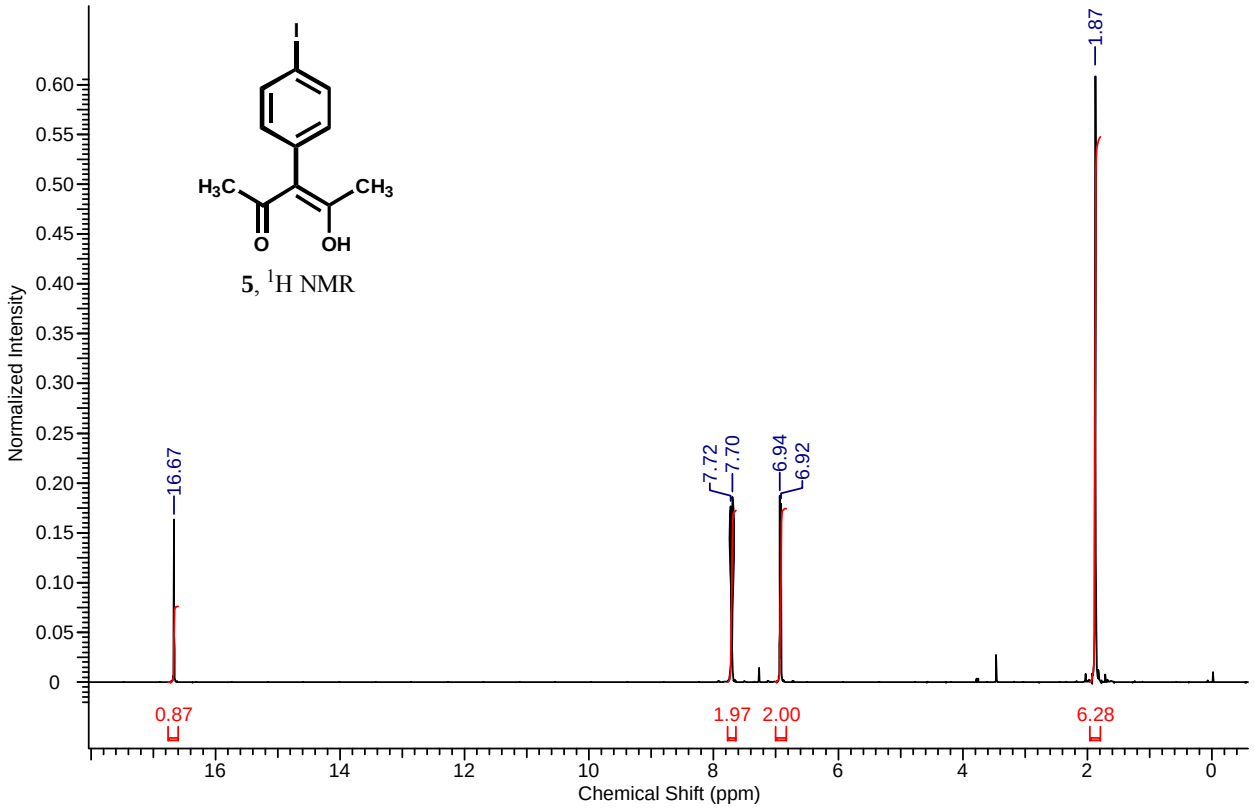
130.86
129.47
114.96
77.32
77.00
76.68
24.14
21.17

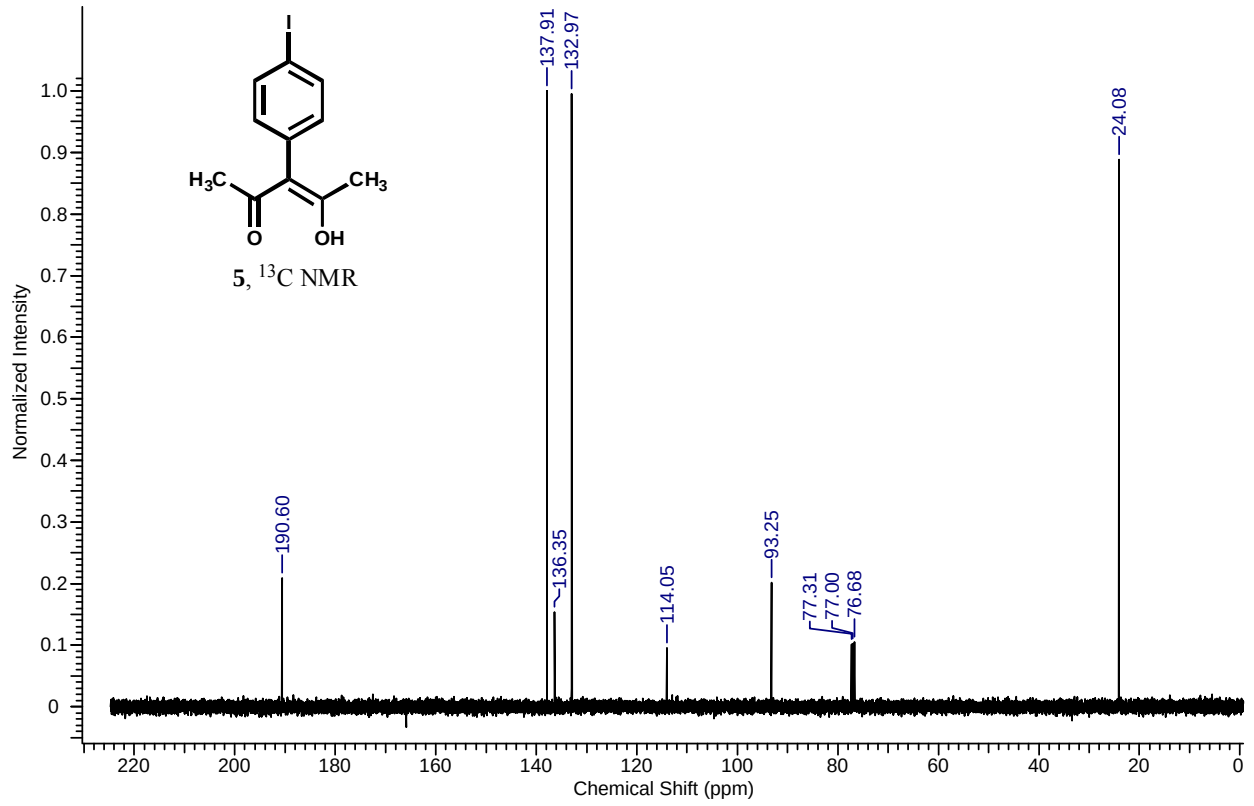









H3C
CH3
O
OH
5, 1H NMR
Normalized Intensity
Chemical Shift (ppm)
16.67
7.72
7.70
6.94
6.92
1.87
0.87
1.97
2.00
6.28


H3C
CH3
O
OH
5, 13C NMR
Normalized Intensity
Chemical Shift (ppm)
190.60
137.91
132.97
136.35
114.05
93.25
77.31
77.00
76.68
24.08